

# Trajectory-constrained optimal local time-continuous waveform controls for state transitions in $N$ -level quantum systems

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Based on a parametrization of pure quantum states we explicitly construct a sequence of (at most)  $4N - 5$  local time-continuous waveform controls to achieve the specified state transition for  $N$ -level quantum system when sufficient controls of the Hamiltonian are available. The control magnitudes are further optimized in terms of the time-energy performance which is the generalization of the time performance, and then the trajectory-constrained optimal local time-continuous waveforms controls including both local sine-waveforms and  $n$ -order-polynomial-function-waveform controls are obtained in terms of time-energy performance. It is demonstrated that constrained optimal local  $n$ st-order-polynomial-function-waveform controls approach constrained optimal bang-bang controls when  $n \rightarrow \infty$ .

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## I. INTRODUCTION

Control of quantum systems has been recognized as an important issue for some time with early beginnings of the application of control theory in the quantum domain dating back to the 1980s [1–3]. Generally, the main goal of control theory is to find controls leading the objects to a desired situation. There are usually two ways of specifying “a desired prescribed situation”: the controllability viewpoint and the optimization viewpoint[4]. The controllability of quantum systems has been investigated by many researchers (see Ref. [1, 5, 6]). Optimal control theory has also been successfully applied to the design of open-loop coherent control strategies in physical chemistry [7, 8]. Recently, time-optimal control problems for spin systems have been solved to achieve specified control objectives in minimum time [9–11]. In general, optimal control problems can only be solved by using numerical optimization techniques.

When sufficient controls of the Hamiltonian are available, the third kind of mixed approach may be adopted: one can first construct some simple controls along a chosen trajectory to achieve a desired state transition, and then make full use of degree of freedom to optimize some kind of performances including minimum time performance. In this way, trajectory-constrained simple optimal controls are obtained. Present technology justifies this third approach for some super-conducting systems [12–14] and nuclear magnetic resonance systems(NMR) [15], for example. It has been demonstrated that simple waveforms such as local square wave function (Bang Bang control) [21] can be constructed to achieve the desired state transition. Quite recently, Bang

Bang control has been successfully applied in some physical systems[16–20]. In practice the control functions need not be restricted to bang-bang controls but other time-continuous function waveforms such as triangle-waveforms and sine-waveform may be used to manipulate quantum states of  $N$ -level quantum systems. In this paper, the third kind of mixed viewpoint is adopted and it is demonstrated that local time-continuous function waveforms including both local  $n$ -order-polynomial waveforms and sine waveforms can be constructed to achieve the desired state transitions.

## II. PREREQUISITE

The state of an  $N$ -level quantum mechanical system is presented by a vector in  $N$ -dimensional Hilbert space  $H$ . In quantum mechanics, the state  $\psi$  is denoted as  $|\psi\rangle$  and called *ket*. To any  $|\psi\rangle$  is associated a linear operator  $\langle\psi| : H \rightarrow C$ , which is called *bra*. Given a *ket*  $|\psi\rangle$  and a *bra*  $\langle\phi|$ , we define a linear operator  $|\psi\rangle\langle\phi| : H \rightarrow H$ . The state of an  $N$ -level quantum system can be expressed as  $|\psi\rangle = \sum_{n=0}^{N-1} c_n |n\rangle$  with regard to a chosen basis  $|n\rangle$  ( $n = 0, 1, 2, \dots, N-1$ ) in the Hilbert space. The coefficients  $c_n$  are a set of complex numbers satisfying the normalization constraint  $\sum_{n=0}^{N-1} |c_n|^2 = 1$ . By ignoring the global phase, the coefficients can be expressed as

$$\begin{pmatrix} c_0 \\ \vdots \\ c_{N-2} \\ c_{N-1} \end{pmatrix} = \begin{pmatrix} \cos \frac{\theta_1}{2} \\ \vdots \\ e^{i\phi_{N-2}} \sin \frac{\theta_1}{2} \dots \sin \frac{\theta_{N-2}}{2} \cos \frac{\theta_{N-1}}{2} \\ e^{i\phi_{N-1}} \sin \frac{\theta_1}{2} \dots \sin \frac{\theta_{N-2}}{2} \sin \frac{\theta_{N-1}}{2} \end{pmatrix} \quad (1)$$

with  $0 \leq \theta_1, \dots, \theta_{N-1} \leq \pi$  and  $0 \leq \phi_1, \dots, \phi_{N-1} < 2\pi$ . Thus any pure state  $|\psi\rangle$  of an  $N$ -level quantum system can be represented by the  $2(N-1)$  generalized geometric parameters  $(\Theta; \Phi)$  with  $\Theta = (\theta_1, \dots, \theta_{N-1})^T$  and  $\Phi = (\phi_1, \dots, \phi_{N-1})^T$ .

For  $N \geq 2$  we define the operators ( $N \times N$  matrices)

$$x_{N,k} = |k\rangle\langle k+1| + |k+1\rangle\langle k| \quad (2a)$$

$$y_{N,k} = i[|k+1\rangle\langle k| - |k\rangle\langle k+1|] \quad (2b)$$

$$z_{N,k} = I_N - 2|k+1\rangle\langle k+1| \quad (2c)$$

$$I_{N,k} = |k\rangle\langle k| + |k+1\rangle\langle k+1|. \quad (2d)$$

for  $k = 0, 1, \dots, N-2$  where  $I_N = \sum_{j=0}^{N-1} |j\rangle\langle j|$  is the identity. For  $N = 2$  these reduce to the standard Pauli operators  $z_{2,0} = \sigma_z$ ,  $y_{2,0} = \sigma_y$  and  $x_{2,0} = \sigma_x$ .

**Lemma:** Let  $0 \leq t_0 < t_1 < \infty$  and  $t \in (t_0, t_1) \subset R^+$ . Both  $F(t)$  and  $f(t)$  are scalar time functions defined on  $R$ . If  $\frac{dF(t)}{dt} = f(t)$  for  $t \in (t_0, t_1)$  and  $H$  is a constant Hamiltonian, then the solution of the operator differential equation

$$i\dot{X}(t) = f(t)HX(t) \quad (3)$$

is given by  $X(t) = e^{-i[F(t)-F(t_0)]H}X(t_0)$  with the initial state  $X(t_0)$ .

Setting  $\Delta F(t) = F(t) - F(t_0)$  evaluation of the matrix exponential for  $H = z_{N,k}$  and  $H = y_{N,k}$  yields the explicit formulas

$$e^{-i\Delta F(t)z_{N,k}} = e^{-i\Delta F(t)}\{I_N + [e^{i2\Delta F(t)} - 1]|k+1\rangle\langle k+1|\} \quad (4a)$$

$$e^{-i\Delta F(t)y_{N,k}} = I_{N,k} \cos \Delta F(t) - iy_{N,k} \sin \Delta F(t) + I_N - I_{N,k}. \quad (4b)$$

This Lemma implies that one have degree of freedom to construct control Hamiltonian to steer the quantum system to the target state. In this paper we focus on controls given by both a local sine waveform

$$f_{ls}(t; t_0, t_1, A) = \begin{cases} A \sin \frac{\pi(t-t_0)}{(t_1-t_0)} & t \in [t_0, t_1] \\ 0 & \text{otherwise} \end{cases} \quad (5)$$

and a local  $n$ -order-polynomial-function  $f_{ln}(t; t_0, t_1, A)$

$$f_{ln}(t; t_0, t_1, A) = \begin{cases} -A \left[ \frac{t_1+t_0-2t}{t_1-t_0} \right]^n + A & t \in [t_0, \frac{t_0+t_1}{2}] \\ -A \left[ \frac{2t-(t_1+t_0)}{t_1-t_0} \right]^n + A & t \in [\frac{t_0+t_1}{2}, t_1] \\ 0 & \text{otherwise} \end{cases} \quad (6)$$

We further have  $\int_{t_0}^{t_1} f_{ls}(t; t_0, t_1, A) dt = \frac{2A(t_1-t_0)}{\pi}$ ,  $\int_{t_0}^{t_1} f_{ln}(t; t_0, t_1, A) dt = \frac{A(t_1-t_0)n}{n+1}$ ,  $\int_0^\infty |f_{ls}(t; t_0, t_1, A)|^2 dt = \frac{A^2(t_1-t_0)}{2}$  and  $\int_0^\infty |f_{ln}(t; t_0, t_1, A)|^2 dt = \frac{A^2(t_1-t_0)2n^2}{2n^2+3n+1}$ .

When some waveform controls are chosen to achieve a state transition at the target time  $t_f$ , we still have some degree of freedom to optimize the control magnitudes with regard to a chosen performance index. Here

we shall consider two kind of performance indices, the transition time  $J_t = \int_0^{t_f} 1 dt = t_f$  and a combined time-energy performance index

$$J_{te} = t_f + \lambda^{-1} \cdot \int_0^{t_f} E(u(t)) dt = \int_0^{t_f} [1 + \lambda^{-1} E(u(t))] dt \quad (7)$$

that takes into account the energy cost  $E(u(t))$  of the control vector  $u(t)$  as well as the time required. For example, if  $H(t) = \sum_i u_i(t) H_i$ , then  $u(t) = (u_i(t))$  and  $E(u(t)) = \sum_i |u_i(t)|^2$ . Here  $\lambda > 0$  is introduced as a ratio parameter that defines the relative weight of the energy and time resource costs, and the equivalent physical unit of  $\lambda$  is  $W = J \cdot s^{-1} = N \cdot m \cdot s^{-1} = (kg) \cdot m^2 \cdot s^{-3}$ . It should be emphasized that  $J_{te}$  is reduced to  $J_t$  if  $\lambda \rightarrow \infty$ , so the time-energy performance  $J_{te}$  can be interrupted as the generalization of time performance.

### III. TRAJECTORY-CONSTRAINED OPTIMAL LOCAL SINE-WAVEFORM TRANSITION CONTROLS

Consider an  $N$ -level quantum system which is governed by the Schrödinger equation (in units of  $\hbar = 1$ )

$$i \frac{d}{dt} |\psi(t)\rangle = \sum_{k=0}^{N-2} [u_{y,k}(t) y_{N,k} + u_{z,k}(t) z_{N,k}] |\psi(t)\rangle \quad (8)$$

where  $y_{N,k}$  and  $z_{N,k}$  are defined in Eq. (2). Such a drift-free Hamiltonian can be obtained for many systems by transforming to a rotating frame, suitably expanding the control fields and making certain simplifying assumptions as discussed e.g. in Ref. [21].

It has been demonstrated in Ref. [21] that one can steer the system (8) from an arbitrary initial state  $|\psi_0\rangle$  to a target state  $|\psi_s\rangle$  by using (at most)  $4N - 5$  Bang-Bang control based on the parametrization of the initial and target states in terms of the  $2(N-1)$  geometric parameters  $(\Theta_0; \Phi_0) = (\theta_1^0, \dots, \theta_{N-1}^0; \phi_1^0, \dots, \phi_{N-1}^0)^T$  and  $(\Theta_s; \Phi_s) = (\theta_1^s, \dots, \theta_{N-1}^s; \phi_1^s, \dots, \phi_{N-1}^s)^T$  described in Section 2. One can also achieve the same state transition by using (at most)  $4N - 5$  local sine waveform controls and the design process can be divided into three stages: (1) Steer the quNit from  $(\Theta_0; \Phi_0)$  to  $(\Theta_0; \mathbf{0})$  by performing  $(N-1)$  local  $Z$ -rotations; (2) Transfer the quNit from  $(\Theta_0; \mathbf{0})$  to  $(\Theta_s; \mathbf{0})$  by performing  $2N-3$  local  $Y$ -rotations; (3) Manipulate the quNit from  $(\Theta_s; \mathbf{0})$  to  $(\Theta_s; \Phi_s)$  by performing  $(N-1)$  local  $Z$ -rotations.

Let  $m = 2, 3, \dots, N-1$  and  $j = 1, 2, \dots, N-1$ , we have

$$\begin{aligned} u_{y,0}(t) &= \text{sgn}(\theta_1^0 - \theta_1^s) f_{ls}(t; t_{2N-3}, t_{2N-2}, A_{\theta_1^0}) \\ u_{y,m-1}(t) &= f_{ls}(t; t_{2N-2-m}, t_{2N-1-m}, A_{\theta_m^0}) y_{N,m-1} \\ &\quad - f_{ls}(t; t_{2N-4+m}, t_{2N-3+m}, A_{\theta_m^s}) y_{N,m-1} \\ u_{z,j-1}(t) &= \text{sgn}(\pi - \phi_j^0) f_{ls}(t; t_{j-1}, t_j, A_{\phi_j^0}) \\ &= \text{sgn}(\phi_j^s - \pi) f_{ls}(t; t_{3N-5+j}, t_{3N-4+j}, A_{\phi_j^s}) \end{aligned} \quad (9)$$

with control magnitudes  $A_{\theta_m^0}, A_{\theta_m^s}, A_{\theta_1^0}, A_{\phi_j^0}$ , and  $A_{\phi_j^s}$  corresponding to the geometric parameter  $\theta_m^0, \theta_m^s, \theta_1^0 - \theta_1^s, \phi_j^0$  and  $\phi_j^s$ .  $t_j - t_{j-1} = \frac{\min\{\phi_j^0, 2\pi - \phi_j^0\}\pi}{4A_{\phi_j^0}} t_{2N-1-m} - t_{2N-2-m} = \frac{\theta_m^0 \cdot \pi}{4A_{\theta_m^0}}, t_{2N-2} - t_{2N-3} = \frac{|\theta_1^0 - \theta_1^s| \cdot \pi}{4A_{\theta_1^0}}, t_{2N-3+j} - t_{2N-4+j} = \frac{\theta_j^s \cdot \pi}{4A_{\theta_j^s}}$  and  $t_{3N-4+j} - t_{3N-5+j} = \frac{\min\{2\pi - \phi_j^s, \phi_j^s\}\pi}{4A_{\phi_j^s}}$

Both the transition time  $t_f = t_{4N-5} - t_0$  and the corresponding energy cost can be expressed in terms of the initial and target state parameters as well as the magnitudes of sine waveform functions. This implies that one can optimize the magnitudes of sine wave function in terms of time-energy performance index given by Eq. (7).

Suppose the control amplitudes are bounded by  $L$ , and denote  $L_s^* = \min(L, \sqrt{2\lambda})$  and  $w_{ls}(x) = \frac{\pi}{4}(\frac{1}{x} + \frac{x}{2\lambda})$ , the optimal amplitudes for the sine waveform controls, minimizing the performance index  $J_{te}$ , are  $A_{\phi_j^0} = A_{\phi_j^s} = A_{\theta_m^0} = A_{\theta_m^s} = A_{\theta_1^0} = L_s^*$  and we have

$$J_{te}^* = t_f + \lambda^{-1} \cdot \int_0^{t_f} E(u(t))dt = (C_1 + C_2)w_{ls}(L_s^*) \quad (10)$$

where  $C_1$  and  $C_2$  are given by

$$\begin{aligned} C_1 &= \sum_{l=2}^{N-1} (\theta_l^0 + \theta_l^s) + |\theta_1^0 - \theta_1^s| \\ C_2 &= \sum_{k=1}^{N-1} [\min(2\pi - \phi_k^0, \phi_k^0) + \min(2\pi - \phi_k^s, \phi_k^s)]. \end{aligned} \quad (11)$$

The “best” time performance for bounded controls is obtained by letting  $\lambda \rightarrow +\infty$ . If  $L \rightarrow +\infty$ , then time performance index  $J_t \rightarrow 0$ .

To intuitively understand the aforementioned analysis, we further consider a concrete example by setting  $N = 2$ ,  $|\psi_0\rangle = |0\rangle$ ,  $|\psi_s\rangle = \frac{\sqrt{2}}{2}|0\rangle + i\frac{\sqrt{2}}{2}|1\rangle$ ,  $\lambda = 2$  and  $L = 1$ . For this concrete example,  $J_{te}^* = \frac{5\pi^2}{16}$  and the corresponding constrained optimal bounded sine-waveform controls are given as follow

$$\begin{aligned} u_z^*(t) &= \begin{cases} -\sin \frac{8t - \pi^2}{\pi} & t \in [\frac{\pi^2}{8}, \frac{\pi^2}{4}] \\ 0 & \text{otherwise} \end{cases} \\ u_y^*(t) &= \begin{cases} \sin \frac{8t}{\pi} & t \in [0, \frac{\pi^2}{8}] \\ 0 & \text{otherwise} \end{cases} \end{aligned} \quad (12)$$

This implies that the desired state transition is achieved by 2-rotations as shown in Fig.1(a). One can also achieve the same state transition along one-rotation trajectory (Fig.1(b)) by choosing

$$u_z^*(t) = u_y^*(t) = \begin{cases} \sin \frac{4\sqrt{2}t}{\pi} & t \in [0, \frac{\sqrt{2}\pi^2}{8}] \\ 0 & \text{otherwise} \end{cases} \quad (13)$$

and the corresponding time-energy performance is  $J_{te}^* = \frac{3\sqrt{2}\pi^2}{16}$ . Therefore, it is exemplified that the obtained optimal sine-waveform controls proposed in this section are

TABLE I: Trajectory-constrained minimum transition times  $J_t$  for bounded controls with amplitude bounds given by  $L$  and optimal time-energy performance  $J_{te}$  for both bounded and unbounded controls for different waveforms.

Case	$J_t$	$J_{te}(\text{bounded})$	$J_{te}(\text{unbounded})$
BB	$\frac{1}{2}t_*$	$w_{lb}(L_B^*)(C_1 + C_2)$	$\sqrt{\lambda}(C_1 + C_2)$
LN	$\frac{n+1}{2n}t_*$	$w_{ln}(L_n^*)(C_1 + C_2)$	$\frac{\sqrt{(2n+1)(2n+2)\lambda}}{2n}(C_1 + C_2)$
LS	$\frac{\pi}{4}t_*$	$w_{ls}(L_s^*)(C_1 + C_2)$	$\frac{\pi\sqrt{2\lambda}}{4}(C_1 + C_2)$

not globally optimal because they are subject to constraints on the control waveforms and trajectories. It should be also underlined in the aforementioned example that one can generate the target state  $|\psi_s\rangle = \frac{\sqrt{2}}{2}|0\rangle + i\frac{\sqrt{2}}{2}|1\rangle$  at  $t_k = \frac{\sqrt{2}\pi^2}{8} + \frac{k\sqrt{2}\pi^2}{4}$  ( $k = 0, 1, 2, \dots$ ) by performing the sine waveform functions  $u_z^*(t) = u_y^*(t) = \sin \frac{4\sqrt{2}t}{\pi}$  on the controlled qubit.

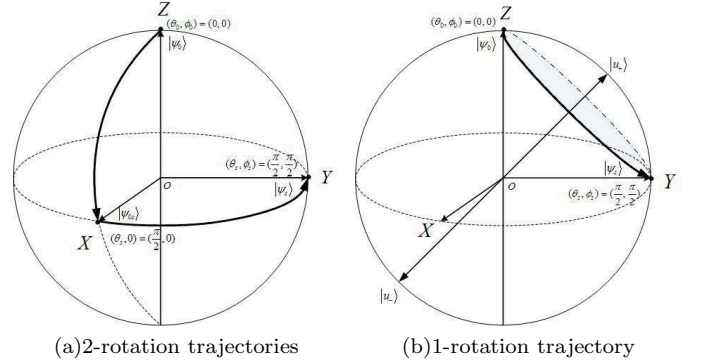


FIG. 1: Two kinds of trajectories on the Bloch sphere

#### IV. DISCUSSION AND CONCLUSION

Following similar analysis as in Section 3, one can obtain trajectory-constrained optimal  $n$ st-order polynomial waveform controls. Denote  $w_{lb}(x) = \frac{1}{2}(\frac{1}{x} + \frac{x}{\lambda})$ ,  $w_{ln}(x) = (\frac{n+1}{2nx} + \frac{nx}{(2n+1)\lambda})$ ,  $L_B^* = \min(L, \sqrt{\lambda})$ ,  $L_n^* = \min(L, \frac{\sqrt{(2n+1)(2n+2)\lambda}}{2n})$  and  $t_* = (C_1 + C_2)/L$  with constants  $C_1$  and  $C_2$  defined as Eq. (11). The time and time-energy performances are further summered in Table I for constrained optimal Bang-Bang (BB) controls, constrained optimal local sine-waveform (LS) controls, and constrained optimal local  $n$ -order-polynomial-function-waveforms(LN) controls.

In this technical communique, we utilize the geometric parametrization of quantum states and the properties of generalized Pauli operators to develop analytic control schemes and then construct optimal local time-continuous function controls to achieve state transitions for multi-level quantum systems. We use the remain-

ing degrees of freedom to optimize the magnitude parameters of the time-continuous function with regard to time-energy performance. Constrained optimal controls of both sine-waveform and  $n$ -order-polynomial-function-waveform are obtained. When  $n \rightarrow \infty$ , constrained optimal LN controls approach to the constrained optimal BB controls, generalizing the results in [21].

The choice of a time-energy performance index given by Eq. (7) is motivated by experimental feasibility considerations, which require that the desire for fast state transition be balanced against the need to limit the amount of energy required to achieve the transition. It should be underlined that Eq. (7) is reduced to  $J_t$  when  $\lambda \rightarrow \infty$ , therefore time-energy performance can be interpreted as a generalization of time performance.

Although the trajectory-constrained optimal time-continuous waveform controls are not globally optimal, the resulting constrained optimal controls have the advantage of being of a simple form, which can be given analytically without the burden for numerical optimization. It is also exemplified in section 3 that periodic sine waveform controls could possibly be utilized to periodically generate the target state, and this observation implies that bounded control with finite frequencies can be used for quantum state engineering.

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